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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS	6	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS	7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS	8	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS	9	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS	10	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS	11	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS	12	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS	13	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS	14	DEC 18	CA/CAplus patent kind codes updated
NEWS	15	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS	16	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS	17	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS	18	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS	19	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS	20	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS	21	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS	22	JAN 22	CA/CAplus updated with revised CAS roles
NEWS	23	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS	24	JAN 29	PHAR reloaded with new search and display fields
NEWS	25	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS	26	FEB 13	CASREACT coverage to be extended
NEWS	27	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS	28	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS	29	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS	30	FEB 26	MEDLINE reloaded with enhancements
NEWS	31	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS	32	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS	33	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS	34	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS	35	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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 NEWS HOURS     STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN     Welcome Banner and News Items
 NEWS IPC8      For general information regarding STN implementation of IPC 8
 NEWS X25       X.25 communication option no longer available

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                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

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=>
Uploading C:\Program Files\Stnexp\Queries\9312351-specific-broad2.str

L1      STRUCTURE UPLOADED

=> s l1 full
FULL SEARCH INITIATED 09:51:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     5315 TO ITERATE

100.0% PROCESSED     5315 ITERATIONS                          33 ANSWERS
SEARCH TIME: 00.00.01

L2           33 SEA SSS FUL L1
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=> file caplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       172.10     172.31

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FILE LAST UPDATED: 14 Mar 2007  (20070314/ED)

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=> s l2
L3           35 L2

=> s l2 not py > 1998
             35 L2
        8637496 PY > 1998
L4           30 L2 NOT PY > 1998

=> s l2 not PY > 1997
             35 L2
        9437846 PY > 1997
L5           30 L2 NOT PY > 1997

=> d l5 ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 30 ANSWERS - CONTINUE? Y/(N):y

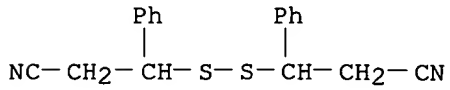
L5   ANSWER 1 OF 30  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         1991:152852  CAPLUS
DOCUMENT NUMBER:          114:152852
TITLE:                    Use of carbon-sulfur cathodes in electroorganic
                          chemistry.  Part 2.  Reactions with activated alkenes.
                          Evidence for a vicarious substitution specific of this
                          type of electrode
AUTHOR(S):                Le Guillanton, G.; Do, Q. T.; Simonet, J.
CORPORATE SOURCE:         Lab. Electrochim. Org., Univ. Cathol. Ouest, Angers,
                          49005, Fr.
SOURCE:                   Bulletin de la Societe Chimique de France (1990),
                          (May-June), 427-39
                          CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE:            Journal
LANGUAGE:                 French
AB   The sulfur-carbon electrode, used as a cathode, appears to be an excellent
     source of nucleophiles which are good sulfuration reagents towards alkenes
     not substituted by leaving groups.  However, the electrochem. reactions
```

are often complex. It should be worth outlining that reaction leads to a vicarious substitution apparently specific of this kind of electrode.

IT 132843-50-6P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. reduction of cyanonitrile on carbon-sulfur electrode)

RN 132843-50-6 CAPLUS

CN Benzenepropanenitrile, β,β'-dithiobis- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:67165 CAPLUS

DOCUMENT NUMBER: 106:67165

TITLE: The preparation of aza-β-lactam, 1,3,4-thiadiazine, β-lactam, and 1,3,4-thiadiazepine derivatives by the reaction of thiosemicarbazides with α- and β-haloacyl halides

AUTHOR(S): Okawara, Tadashi; Kato, Rie; Yamasaki, Tetsuo; Yasuda, Naohiko; Furukawa, Mitsuru

CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan

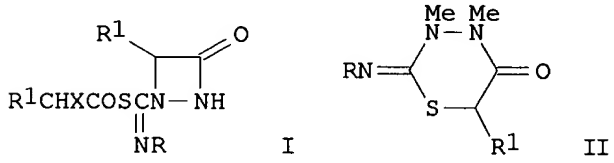
SOURCE: Heterocycles (1986), 24(4), 885-8
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:67165

GI



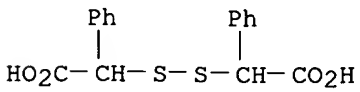
I II

AB RNHC(:S)NHNH2 (R = Me, Bu, cyclohexyl, PhCH2, Ph) reacted with R1CHR2COR2 (R1 = H, Me, R2 = Cl, Br) under two phase conditions to give azalactam I in 44-84% yields. RNHC(:S)NMeNHMe (R = cyclohexyl, Ph, α-naphthyl) reacted with R1CHXCOX (R1 = H, Et, Me, Ph; X = Cl, Br) under the same conditions to give thiadiazinones II in 52-81% yields. I and II cause the differentiation of Friend leukemia cells.

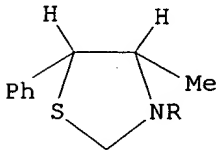
IT 4695-07-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 4695-07-2 CAPLUS

CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)

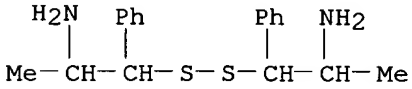


L5 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:504653 CAPLUS
DOCUMENT NUMBER: 99:104653
TITLE: Carbon-13 NMR spectra of β-aminothiols, disulfides and thiazolidines related to thioephedrine
AUTHOR(S): Kone, B.; Gelbcke, M.
CORPORATE SOURCE: Lab. Chim. Pharm. Org. Bromatol., Univ. Libre Bruxelles, Brussels, B-1050, Belg.
SOURCE: Bulletin des Societes Chimiques Belges (1983), 92(3), 203-13
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: French
GI

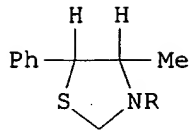


I

AB The 13C NMR spectra of erythro- and threo-PhCH(SH)CH(NHR)Me (R = H, Me, Et, Me2CH, Me3C), diastereoisomers of [MeCH(NHR)CHPh]2 (same R), and diastereoisomers of I (same R) were recorded. The results were discussed in terms of conformations of the diastereoisomers.
IT 86051-01-6
RL: PRP (Properties)
(carbon-13 NMR spectrum and conformation of)
RN 86051-01-6 CAPLUS
CN Benzeneethanamine, β,β'-dithiobis[α-methyl- (9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:421638 CAPLUS
DOCUMENT NUMBER: 99:21638
TITLE: Proton NMR spectra of β-amino thiols, disulfides and thiazolidines related to thioephedrine
AUTHOR(S): Kone, B.; Gelbcke, M.
CORPORATE SOURCE: Inst. Pharm., UNiv. Libre de Bruxelles, Brussels, B-1050, Belg.
SOURCE: Bulletin des Societes Chimiques Belges (1983), 92(2), 139-49
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



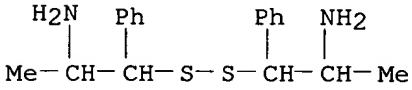
I

AB Diastereoisomers of β-amino thiols PhCH(SH)CHMeNHR (R = H, Me, Et, Me2CH, Me3C), of disulfides PhCH(CHMeNHR)SSCHPhCHMeNHR (same R), and of thiazolidine I (same R) were differentiated by 1H NMR spectra. Conformations of the isomers were discussed in terms of coupling consts.

IT 86051-01-6
RL: PRP (Properties)
(diastereoisomerism and conformation of, NMR in relation to)

RN 86051-01-6 CAPLUS

CN Benzeneethanamine, β,β'-dithiobis[α-methyl- (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:67932 CAPLUS

DOCUMENT NUMBER: 96:67932

TITLE: Chiroptical properties of 2,2'-dithio- and 2,2'-diselenobisacetic acids

AUTHOR(S): Ringdahl, Bjoern; Craig, J. Cymerman; Fredga, Arne; Bonner, William A.

CORPORATE SOURCE: Sch. Pharm., Univ. California, San Francisco, CA, 94143, USA

SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1981), B35(7), 467-71
CODEN: ACBOCV; ISSN: 0302-4369

DOCUMENT TYPE: Journal

LANGUAGE: English

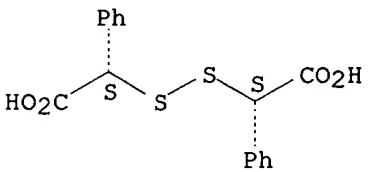
AB CD studies of 2,2'-dithiobisacetic acids substituted with alkyl or Ph groups and their diselenide analogs show that considerable interaction occurs between the disulfide(or diselenide) chromophore and the carboxyl or Ph groups, giving rise to intense Cotton effects (CE) which dominate the near UV region of the CD spectrum. In contrast, when the disulfide and carboxyl chromophores are separated by two C atoms, each chromophore gives a sep. CE of normal intensity at the expected wavelength with no evidence of interaction between them.

IT 16201-54-0
RL: PRP (Properties)
(CD spectrum of)

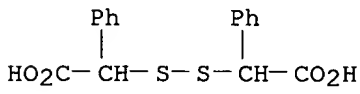
RN 16201-54-0 CAPLUS

CN Benzeneacetic acid, α,α'-dithiobis-, [S-(R*,R*)]- (8CI, 9CI) (CA INDEX NAME)

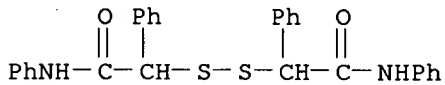
Absolute stereochemistry.



L5 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:615312 CAPLUS
DOCUMENT NUMBER: 89:215312
TITLE: Synthesis of 1,3-dithiolylium salts and reactions of mesoionic 1,3-dithiolones with amines
AUTHOR(S): Gotthardt, Hans; Weisshuhn, C. Michael
CORPORATE SOURCE: Gesamthochsch. Wuppertal, Wuppertal, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1978), 111(9), 3178-82
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 89:215312
GI For diagram(s), see printed CA Issue.
AB Treating R1CS2CHRCO2H (R = H, Ph; R1 = Ph, SEt, p-tolyl) with Ac2O in the presence of acids gave dithiolium salts I (X = ClO4, HSO4) which in polar solvents are easily cleaved to II. Nucleophilic attack of morpholine on II (R = Ph, R1 = Ph, p-tolyl) gave R1CSR2 (R2 = morpholino) and (R2COCHPhS)2. Treating II (R = R1 = Ph) with PhNH2 gave 76% III as well as PhCSNHPh (5%) and (PhNHCOCHPhS)2 (9%).
IT 4695-07-2P 68145-28-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 4695-07-2 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)



RN 68145-28-8 CAPLUS
CN Benzeneacetamide, α,α'-dithiobis[N-phenyl- (9CI) (CA INDEX NAME)



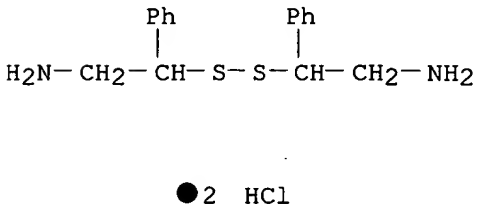
L5 ANSWER 7 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:31877 CAPLUS
DOCUMENT NUMBER: 88:31877
TITLE: Studies on chemical protectors against radiation. XVII. Radioprotective activities of phenethylamine compounds
AUTHOR(S): Shinoda, Masato; Ohta, Setsuko; Takagi, Yoshinari
CORPORATE SOURCE: Hoshi Coll. Pharm., Tokyo, Japan
SOURCE: Yakugaku Zasshi (1977), 97(10), 1117-24
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB The relation between chemical structure and radioprotective activity was examined with 80 phenethylamine compds. and various amines. A strong radioprotective effect was shown by phenethylamine-HCl [156-28-5] and by tyramine-HCl [60-19-5], dopamine-HCl [62-31-7], norepinephrine [51-41-2], and epinephrine-HCl [55-31-2], which have a phenolic hydroxyl in their mol., but the corresponding amino acids were ineffective. Only a weak effect was shown by the ephedrine isomers, but a markedly strong effect was shown by compds. with a side chain substituted with SH,

isothiourea, or thiosulfuric acid, and by the S-S ephedrine compds. Comparison of the isomers of these compds. showed that the L-erythro type compds. were more effective.

IT 3907-60-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(radioprotective activity of)

RN 3907-60-6 CAPLUS

CN Benzeneethanamine, β,β'-dithiobis-, dihydrochloride (9CI) (CA INDEX NAME)



L5 ANSWER 8 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:166353 CAPLUS

DOCUMENT NUMBER: 86:166353

TITLE: Alteration of O,O-dimethyl S-[α-(carboethoxy)benzyl] phosphorodithioate (phenthoate) in citrus, water, and upon exposure to air and sunlight

AUTHOR(S): Takade, Dennis Y.; Seo, Myung-Soo; Kao, T. S.; Fukuto, T. R.

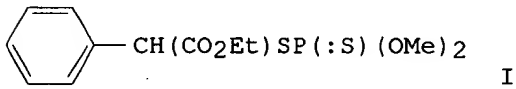
CORPORATE SOURCE: Dep. Entomol., Univ. California, Riverside, CA, USA

SOURCE: Archives of Environmental Contamination and Toxicology (1976), 5(1), 63-86
CODEN: AECTCV; ISSN: 0090-4341

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



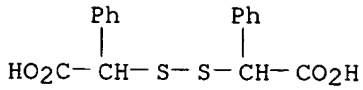
I

AB The fate of 32P- and 14C-labeled phenthoate (O,O-dimethyl S-[α-(carboethoxy)benzyl] phosphoroddithioate)(I) [2597-03-7] was determined in citrus, water, and upon exposure to air and sunlight. The products recovered from citrus and glass plates exposed to sunlight were unchanged I, phenthoate oxon [3690-28-6], demethyl phenthoate [62488-69-1], mandelic acid [90-64-2], bis-[α-(carboethoxy)benzyl] disulfide [36519-38-7], O,O-dimethyl phosphorothioic acid [1112-38-5], and phosphorodithioic acid [15834-33-0]. Similar products generally were found in citrus leaf and fruit exts. I was fairly stable in phosphate-buffered water with a half-life of approx. 12 days at pH 8.0. The major hydrolysis products were phenthoate acid [13376-78-8], demethyl phenthoate and demethyl phenthoate oxon [62488-70-4].

IT 4695-07-2
RL: BIOL (Biological study)
(phenthoate metabolite)

RN 4695-07-2 CAPLUS

CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:577089 CAPLUS
DOCUMENT NUMBER: 85:177089
TITLE: 3-Chlorophenylacetic acid compounds and derivatives
INVENTOR(S): Diamond, Julius; Santora, Norman J.
PATENT ASSIGNEE(S): William H. Rorer, Inc., USA
SOURCE: U.S., 20 pp. Division of U.S. 3,864,384.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 11
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3969401	A	19760713	US 1973-388292	19730814
US 3864384	A	19750204	US 1970-34870	19700505
ES 390860	A1	19730701	ES 1971-390860	19710504
FR 2100632	A5	19720324	FR 1971-16258	19710505
FR 2100632	B1	19751226		
GB 1355681	A	19740605	GB 1971-13150	19710505
CH 563333	A5	19750630	CH 1971-6621	19710505
CH 565760	A5	19750829	CH 1974-6182	19710505
CA 992075	A1	19760629	CA 1971-112243	19710505
FR 2128277	A6	19721020	FR 1971-44544	19711210
ZA 7201348	A	19740327	ZA 1972-1348	19720229
US 3825587	A	19740723	US 1972-233704	19720310
US 3825553	A	19740723	US 1972-233705	19720310
US 3867435	A	19750218	US 1972-233717	19720310
FR 2279387	A2	19760220	FR 1975-8271	19750317
CA 1017749	A2	19770920	CA 1976-248088	19760317

PRIORITY APPLN. INFO.:

US 1970-34870	A3	19700505
US 1971-122998	A	19710310
CA 1971-112243	A3	19710505
US 1971-164920	A	19710721

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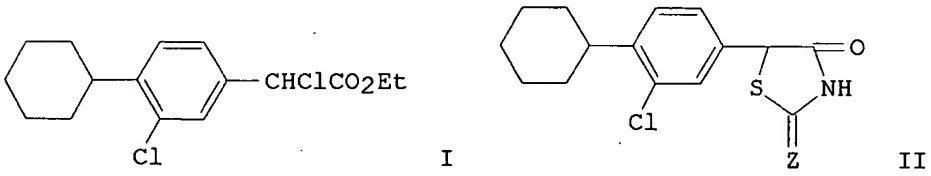


I II

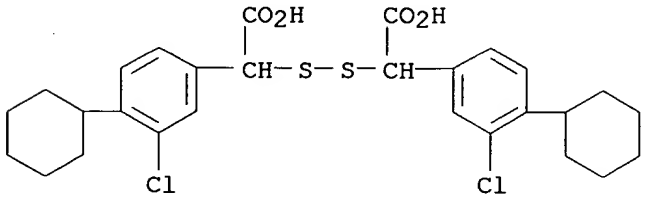
AB 3-Chlorophenylacetic acid derivs., e.g., I and II (Z = NH, O), having antiinflammatory, analgesic, and antipyretic activity, were prepared Thus, Et m-chloro-p-cyclohexylphenylglycolic acid and SOCl2 were stirred 24 hr at room temperature and refluxed 6 hr to give 97.9% I. I and thiourea in EtOH were refluxed 26 hr to give 64.3% II (Z = NH), which was refluxed with 48% HBr to give 51% II (Z = O).

IT 36612-28-9P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and pharmacol. properties of)
RN 36612-28-9 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis[3-chloro-4-cyclohexyl-, compd. with N-ethylethanamine (1:2) (9CI) (CA INDEX NAME)

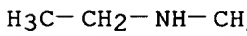
CM 1

CRN 47776-59-0
CMF C28 H32 Cl2 O4 S2

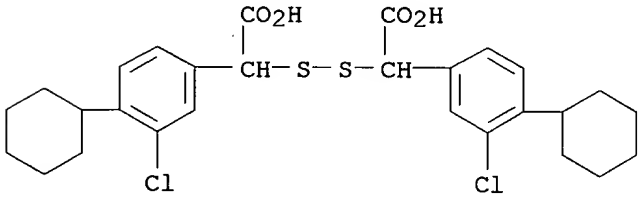


CM 2

CRN 109-89-7
CMF C4 H11 N



IT 47776-59-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 47776-59-0 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis[3-chloro-4-cyclohexyl- (9CI) (CA INDEX NAME)



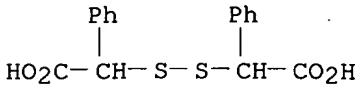
L5 ANSWER 10 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:538239 CAPLUS
DOCUMENT NUMBER: 85:138239
TITLE: Metabolism of O,O-dimethyl S-[α-(carboethoxy)benzyl]phosphorodithioate (phenthoate) in the white mouse and house flies
AUTHOR(S): Takade, Dennis Y.; Allsup, Thurman; Khasawinah, Abdallah; Kao, T. S.; Fukuto, T. R.
CORPORATE SOURCE: Dep. Entomol., Univ. California, Riverside, CA, USA
SOURCE: Pesticide Biochemistry and Physiology (1976), 6(4), 367-76
CODEN: PCBPBS; ISSN: 0048-3575
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The metabolism of phenthoate [2597-03-7], an organophosphorus insecticide of

low mammalian toxicity, was investigated in white mice and in susceptible and resistant strains of houseflies. Phenthoate was metabolized rapidly in the mouse to a wide variety of detoxication products and only an insignificant amount of phenthoate oxon [3690-28-6] was detected. The same detoxication products were produced in houseflies but compared, to the mouse, substantial amts. of phenthoate oxon also were found. The selective toxicity of phenthoate between insect and mammal is attributable to the difference in the accumulation of the oxon.

IT 4695-07-2
RL: FORM (Formation, nonpreparative)
(formation of, as phenthoate metabolite, in insects and mammals)

RN 4695-07-2 CAPLUS

CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)



L5 ANSWER 11 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1974:504187 CAPLUS

DOCUMENT NUMBER: 81:104187

TITLE: NMR spectroscopy of meso and racemic forms of compounds with two equivalent asymmetric carbon atoms in an open chain

AUTHOR(S): Larsson, Erik

CORPORATE SOURCE: Chem. Inst., Univ. Lund, Lund, Swed.

SOURCE: Organic Magnetic Resonance (1974), 6(2), 103-5
CODEN: ORMRBD; ISSN: 0030-4921

DOCUMENT TYPE: Journal

LANGUAGE: German

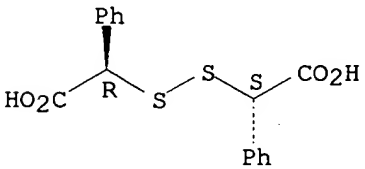
AB Chemical shifts for CH and OMe protons for meso and racemic compds. (RCHCO2H)2, (R = Cl, Br, PhS, MeCOS), (PhCHCO2H) 2S, and (PhCHCO2H)S2 and their Me esters, in a number of solvents. The magnitude of chemical shifts of the meso forms did not correlate with those of the racemic forms, and relative configurations could not be assigned on that basis. The difference in spectra between meso and racemic forms was sufficient to allow their determination in admixt.

IT 53318-27-7 53318-28-8
RL: PRP (Properties)
(NMR of)

RN 53318-27-7 CAPLUS

CN Benzeneacetic acid, α,α'-dithiobis-, (R*,S*)- (9CI) (CA INDEX NAME)

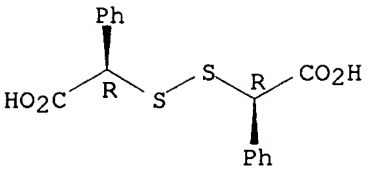
Relative stereochemistry.



RN 53318-28-8 CAPLUS

CN Benzeneacetic acid, α,α'-dithiobis-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L5 ANSWER 12 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:419390 CAPLUS
DOCUMENT NUMBER: 77:19390
TITLE: Antiinflammatory, analgesic, and antipyretic substituted phenylacetic acid compounds
INVENTOR(S): Diamond, Julius; Santora, Norman J.
PATENT ASSIGNEE(S): William H. Rorer, Inc.
SOURCE: Ger. Offen., 91 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 11
PATENT INFORMATION:

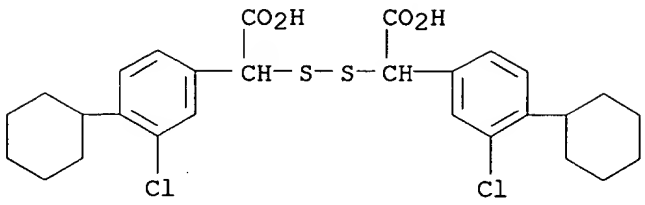
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2122273	A1	19720316	DE 1971-2122273	19710503
DE 2122273	B2	19771229		
US 3864384	A	19750204	US 1970-34870	19700505
ES 390860	A1	19730701	ES 1971-390860	19710504
FR 2100632	A5	19720324	FR 1971-16258	19710505
FR 2100632	B1	19751226		
GB 1355681	A	19740605	GB 1971-13150	19710505
CH 563333	A5	19750630	CH 1971-6621	19710505
CH 565760	A5	19750829	CH 1974-6182	19710505
CA 992075	A1	19760629	CA 1971-112243	19710505
FR 2128277	A6	19721020	FR 1971-44544	19711210
ZA 7201348	A	19740327	ZA 1972-1348	19720229
US 3825587	A	19740723	US 1972-233704	19720310
US 3825553	A	19740723	US 1972-233705	19720310
US 3867435	A	19750218	US 1972-233717	19720310
FR 2279387	A2	19760220	FR 1975-8271	19750317
CA 1017749	A2	19770920	CA 1976-248088	19760317
PRIORITY APPLN. INFO.:			US 1970-34870 A	19700505
			US 1971-122998 A	19710310
			CA 1971-112243 A3	19710505
			US 1971-164920 A	19710721

GI For diagram(s), see printed CA Issue.
AB I (R = H or Me; Y = Cl or Br) were prepared from the corresponding glycolic acid by treatment with SOCl2 and PBr5 and the reaction of I with Et2NH, Me2NH, and NaHCO3 gave the carboxylate salts. Also prepared were the thiazolidines II (R = H or Me; X = NH or O) and the disulfide derivative III. I, II, and III showed antiinflammatory, analgesic, and antipyretic activity in male rats.
IT 36612-28-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36612-28-9 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis[3-chloro-4-cyclohexyl-, compd. with N-ethylethanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

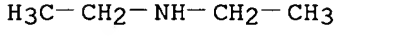
CRN 47776-59-0

CMF C28 H32 Cl2 O4 S2

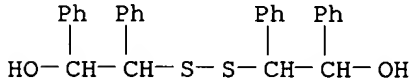


CM 2

CRN 109-89-7
CMF C4 H11 N



L5 ANSWER 13 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:85121 CAPLUS
DOCUMENT NUMBER: 76:85121
TITLE: Reductions with sulfurated borohydrides. VII. Reactions with epoxides
AUTHOR(S): Lalancette, J. M.; Freche, A.
CORPORATE SOURCE: Fac. Sci., Univ. Sherbrooke, Sherbrooke, QC, Can.
SOURCE: Canadian Journal of Chemistry (1971), 49(24), 4047-53
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Reaction of NaBH2S3 with epoxides gives sym. bis(2-hydroxyethyl) disulfides. The stereochemistry of the reaction is similar to the attack of H2S on the epoxides in basic solution Substituted epoxides are opened from the less hindered side. The reaction proceeds with good yield and is general. An improved method of preparation of the 1,2-mercaptols is presented.
IT 35034-31-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35034-31-2 CAPLUS
CN Benzeneethanol, β,β'-dithiobis[α-phenyl- (9CI) (CA INDEX NAME)



L5 ANSWER 14 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:551488 CAPLUS
DOCUMENT NUMBER: 75:151488
TITLE: Reductions with sulfurated borohydrides. VI. Reduction of nitro, nitrile, amide, and nitroso groups
AUTHOR(S): Lalancette, J. M.; Brindle, J. R.
CORPORATE SOURCE: Fac. Sci., Univ. Sherbrooke, Sherbrooke, QC, Can.
SOURCE: Canadian Journal of Chemistry (1971), 49(18), 2990-5
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal

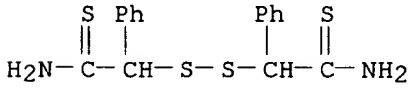
LANGUAGE: English

AB Aromatic nitro compds. can be reduced with sulfurated sodium borohydride to the corresponding amine in high yields (≈80%) without affecting ester, nitrile, ether, halide or olefinic groups also present. With ortho-substituted nitro compds. the yields are around 60%. Primary aliphatic nitro compds. are reduced to the corresponding nitrile in high yields. Secondary aliphatic nitro compds. are reduced to mixts. of ketones and the corresponding oxime. Tertiary aliphatic nitro compds. are not reduced. Aromatic nitriles can be reduced to the corresponding amines with an excess of the reducing agent or converted to the corresponding thioamides with an excess of the nitrile. Amides and nitroso can be reduced to the corresponding amines in moderate yields.

IT 34251-53-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 34251-53-1 CAPLUS

CN Acetamide, 2,2'-dithiobis[2-phenylthio- (8CI) (CA INDEX NAME)



L5 ANSWER 15 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1971:419488 CAPLUS

DOCUMENT NUMBER: 75:19488

TITLE: Alkaline decomposition of organic disulfides. V. Experimental variants of α-elimination

AUTHOR(S): Danehy, James P.; Elia, Victor J.

CORPORATE SOURCE: Dep. Chem., Univ. Notre Dame, Notre Dame, IN, USA

SOURCE: Journal of Organic Chemistry (1971), 36(10), 1394-8
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

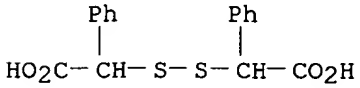
LANGUAGE: English

AB Several compds., which might have been expected to undergo α-elimination in aqueous alkaline solution, failed to give the anticipated mixts. of thiol, carbonyl compound, and H2S. Rather, fairly stable hemidithioketals were formed, apparently by the rapid conversion of the initially formed carbanions into stable thiolate anions. meso-1,2-Dithiane-3,6-dicarboxylic acid (I) in 0.1N NaOH was transformed into trans-2-mercaptothiolane-2,5-dicarboxylic acid about 100 times as rapidly as the corresponding racemic disulfide was transformed into the cis isomer. The bicyclic anhydride of I decomposed at pH 8.6 in the same fashion, but even faster than did I in 0.1N NaOH. The diethyl ester of I is about as sensitive to alkali as is the anhydride. Dithiodisuccinic acid decomposed predominantly by the alternative method and to a small extent by α-elimination.

IT 4695-07-2
RL: PRP (Properties)
(dissociation of, mechanism of)

RN 4695-07-2 CAPLUS

CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)



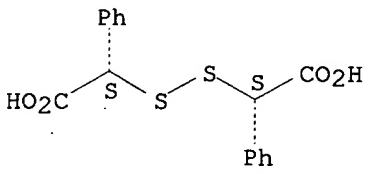
L5 ANSWER 16 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1968:402366 CAPLUS
DOCUMENT NUMBER: 69:2366
TITLE: Preparation, resolution, and absolute configuration of α-mercaptophenylacetic acid
AUTHOR(S): Bonner, William A.
CORPORATE SOURCE: Stanford Univ., Stanford, CA, USA
SOURCE: Journal of Organic Chemistry (1968), 33(5), 1831-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To resolve an ambiguity in the literature, kinetic and stereochem. expts. were undertaken to establish the absolute configuration of α-mercaptophenylacetic acid (I). Polar.acte.imetrically measured second-order rate consts. for the reaction of SH- with Me O-toluenesulfonyl-(S)(+)-mandelate showed a monotonic increase with time, suggesting formation of a strongly levorotatory by-product. When the same reaction was conducted preparatively the desired Me (R)(-)-α-mercaptophenylacetate (68%) was isolated in about 44% optical purity, along with a by-product (32%), (-)-α,α'-bis(carbomethoxy)dibenzyl sulfide, of lower optical purity. S-(Thionocarboethoxy)-α-mercaptophenylacetic acid, prepared by the action of K O-ethyldithiocarbonate on α-chlorophenylacetic acid, was hydrolyzed to yield (±)-I. (±)-I was resolved with the aid of cinchonidine, and was obtained in about 80% optical purity. (-)-I was converted by the action of PhCH2Br and NaHCO3 into (R)(-)-α-benzylthiophenylacetic acid of known absolute configuration, thus confirming the assignment of (-)-I to the (R) series. 21 references.

IT 16201-54-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(alcoholysis of)
RN 16201-54-0 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis-, [S-(R*,R*)]- (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



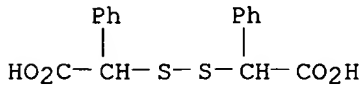
L5 ANSWER 17 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:54721 CAPLUS
DOCUMENT NUMBER: 66:54721
TITLE: Reactions of aryl(trichloromethyl)carbinols with sulfur nucleophiles. Formation and proof of Zwitterionic structure of iminothiazolidinones
AUTHOR(S): Reeve, Wilkins; Nees, Monica
CORPORATE SOURCE: Univ. of Maryland, College Park, MD, USA
SOURCE: Journal of the American Chemical Society (1967), 89(3), 647-51
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB Nucleophilic reagents react with aryl(trichloromethyl)carbinols to give α-substituted acids or derivs. Thiourea acts as a typical nucleophile in this reaction, with a subsequent ring closure giving an iminothiazolidinone. Thus, phenyl(trichloromethyl)carbinol (I) is

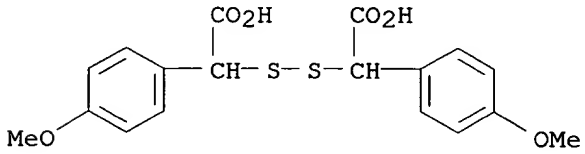
converted in one step to 54% 2-imino-5-phenyl-4-thiazolidinone (II). Similarly are obtained 28% 5-(3,4-dichlorophenyl)-2-imino-4-thiazolidinone and 18% 2-imino-5-(p-methoxyphenyl)-4-thiazolidinone. N.M.R. spectra, together with other evidence, allow the correct structure of the parent iminothiazolidinone to be chosen from the nine possible tautomeric forms. K Me xanthate also functions as a nucleophile in its reaction with I, but CN- does not under the conditions employed. The relative nucleophilicities of the reagents tried are: thiourea » xanthate >MeO » CN.

IT 4695-07-2P 14605-32-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 4695-07-2 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)



RN 14605-32-4 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis[4-methoxy- (9CI) (CA INDEX NAME)



L5 ANSWER 18 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:35831 CAPLUS
DOCUMENT NUMBER: 64:35831
ORIGINAL REFERENCE NO.: 64:6634a-f
TITLE: Effect of sodium hydroxide on several 2,4-thiazolidinediones and 2-imino-4-thiazolidinones. I
AUTHOR(S): Aspelund, Helge
SOURCE: Acta Acad. Aboensis, Math. Phys. (1964), 24(1), 23 pp.
DOCUMENT TYPE: Journal
LANGUAGE: German

GI For diagram(s), see printed CA Issue.

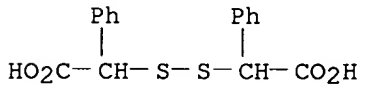
AB cf. CA 59, 3909c. Treatment of thioureas with halo acids, halo acid chlorides, or esters gave the corresponding 2-imino-4-thiazolidinones (I). Acid hydrolysis of I gave 2,4-thiazolidinediones (II). Thus, heating a mixture of 10 g. PhCHClCO2H and 5.4 g. thiourea in 30 ml. PhMe 2.75 hrs. gave I (R = R1 = R3 = H, R2 = Ph) (III), m. 230-1° (decomposition). To a mixture of 8 g. Ph2CClCOCl and 2.8 g. thiourea in 42 ml. AcOH was added 5.6 g. anhydrous AcONa and the mixture heated 2 hrs. to yield 7.2 g. I (R = R1 = H, R2 = R3 = Ph) (IV), m. 282-3°. Similarly were prepared the I shown in the 1st table. Heating 5 g. III.HCl in 6 ml. concentrated H2SO4 and 24 ml. H2O 4.5 hrs. gave II (R1 = R3 = H, R2 = Ph) (XI), m. 127-9°. A mixture of 3 g. PhCHClCO2H and 3.2 g. PhNHCONHMe in 75 ml. toluene was refluxed 3 hrs., cooled, dissolved in ether, washed with alkali and dried. The residue dissolved in alc. was treated with 15 ml. dilute HCl and heated for 2.5 hrs. to give 0.9 g. II (R' = Me, R2 = Ph, R3 = H) (XII), m. 97-8°. Adding 1.8 g. IV and 1 ml. Me2SO4 to MeONa (prepared from 0.225 g. Na in 18 ml. MeOH) and boiling to dryness also yielded XII.

Similarly prepared were the following II (R1, R2, R3, and m.p. given): Ph, Ph, H (III), 171-2°; H, Ph, Ph (XIV), 151-2°; Ph, Ph, Ph (XV), 150-1°; Me, Ph, Ph (XVI), 102°. I and II were treated with 1.2 or 2 equivs. of N NaOH alone or in alc. solution either at 6° or room temperature or under reflux at times ranging from several min. to several hrs. The reaction mixture was then generally extracted with ether, neutralized (and extracted with ether to recover the unreacted I and II), and finally strongly acidified and extracted with ether to obtain acidic reaction products. Thus, a solution of VI in NaOH kept at 6° for 5 days or boiled for 30 min., acidified to pH 4.3, washed with ether (to remove unreacted VI) and then strongly acidified, yielded carbamoylthioglycolic acid, m. 139-40° (decomposition). The following I and II were similarly treated (at reflux temperature, A; room temperature, B; at 6°, C). (Unreacted I and II were present in almost all of the following reactions, but this is indicated only when it is the sole isolated material) (compds., reaction conditions, products, and m.p. given): III, A, diphenyldithiodiglycolic acid (XVII), 208-9°; XI, A, C, PhCH(SCONH2)CO2H, 131-2° (decomposition), and XVII; VII, A, HSCH2CO2H, --; VIII, A, PhCH(SH)CO2H, 62-3°, and diphenylurea (XVIII), 235-6° (decomposition); VIII, B, VIII, --; XIII, A, PhCH(SCONHPh)CO2H, 166-7°, and XVII; XIII, B, PhCH(SH)CO2H (XIX), 58-60°; IV, A, Ph2CHCONH2, 166-7°, and Ph2CHCO2H; XIV, B, resin, --; IX, A, IX, --; X, A, XIX, and XVIII, --; XV, A, diphenylacetanilide, 175-80°, and XVIII and XIX; XV, B, XV, --; XII, A, B, PhCH(SCONHMe)CO2H, 131-2° (decomposition); XVI, A, Ph2C(SH)CONHMe, 101-2°, and XIX; XVI, B, Ph2C(SH)CO2H, 144-8°, and XIX. The stabilities of I and II depended on the substituents and their positions.

IT 4695-07-2P, Acetic acid, dithiobis[phenyl-
RL: PREP (Preparation)
(preparation of)

RN 4695-07-2 CAPLUS

CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)



L5 ANSWER 19 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

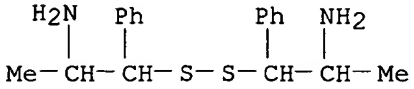
ACCESSION NUMBER: 1965:410292 CAPLUS
DOCUMENT NUMBER: 63:10292
ORIGINAL REFERENCE NO.: 63:1823e-f
TITLE: Nuphamine: A new alkaloid of Nuphar japonicum
AUTHOR(S): Arata, Yoshio; Ohashi, Tsutomu
CORPORATE SOURCE: Univ. Kanazawa, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1965), 13(3), 392-3
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB A new base, nuphamine (I), b3 150-3°, [α]19D -60.48, was isolated from N. japonicum root. Picrolonate m. 159-60°; N-Me methiodide m. 164°. The ir spectrum of I in CCl4 showed bands at 3620, 3150, 1500 cm.-1 I was treated with SOCl2 and the product reduced catalytically to give (-)-deoxynupharamine. Catalytic reduction of I gave a dihydro derivative (II), m. 42.5-3°. N.M.R. spectra of I and II support the proposed structure for I as shown.

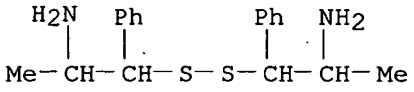
IT 1630-28-0P, Phenethylamine, β,β'-dithiobis[α-methyl-, dihydrobromide 2289-40-9P, Phenethylamine, β,β'-dithiobis[α-methyl-, hydrochloride

RL: PREP (Preparation)
(preparation of)
RN 1630-28-0 CAPLUS
CN Benzeneethanamine, β,β'-dithiobis[α-methyl-, dihydrobromide (9CI) (CA INDEX NAME)



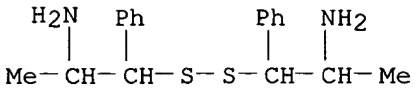
●2 HBr

RN 2289-40-9 CAPLUS
CN Phenethylamine, β,β'-dithiobis[α-methyl-, hydrochloride (8CI) (CA INDEX NAME)



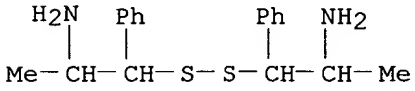
● HCl

L5 ANSWER 20 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:410291 CAPLUS
DOCUMENT NUMBER: 63:10291
ORIGINAL REFERENCE NO.: 63:1823d-e
TITLE: Potential radiation protective agents. IV. Sulfur analogs related to norephedrine
AUTHOR(S): Bhat, K. Venkatramana; McCarthy, Walter C.
CORPORATE SOURCE: Univ. of Washington, Seattle
SOURCE: Journal of Pharmaceutical Sciences (1965), 54(3), 488-9
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. preceding abstract Refluxing 16 g. EtOCS2K, 20.6 g. PhCHClCHMeNH2 (I) HCl salt, 23 ml. 10% MeONa, and 200 ml. anhydrous MeOH for 4 hrs. and subsequent evaporation of the solvent and crystallization of the residue gave 27%
4-methyl-5-phenyl-2-thiazolidinethione, m. 97° (iso-PrOH-cyclohexane). Similarly, 0.172 mole AcSNa refluxed with 0.172 mole I in MeOH produced 5% PhCH(SH)CHMeNHAc (II), m. 151° (dilute EtOH). Air oxidation of II during isolation afforded 22% (AcNHCHMeCHPhS)2 (III), m. 215° (Me2CO), and III refluxed 48 hrs. in concentrated HCl gave 37% (NH2CHMeCHPhS)2, isolated as the di-HBr salt, m. 265-7°.
IT 1630-28-0P, Phenethylamine, β,β'-dithiobis[α-methyl-, dihydrobromide 2289-40-9P, Phenethylamine, β,β'-dithiobis[α-methyl-, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 1630-28-0 CAPLUS
CN Benzeneethanamine, β,β'-dithiobis[α-methyl-, dihydrobromide (9CI) (CA INDEX NAME)



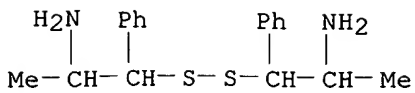
● 2 HBr

RN 2289-40-9 CAPLUS
CN Phenethylamine, β,β'-dithiobis[α-methyl-, hydrochloride (8CI) (CA INDEX NAME)



● HCl

L5 ANSWER 21 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:8904 CAPLUS
DOCUMENT NUMBER: 62:8904
ORIGINAL REFERENCE NO.: 62:1588a-c
TITLE: Phenylmercaptoalkylamines. III. Hofmann degradation of 1-phenyl-2-dimethylaminopropanethiol quaternary salts
AUTHOR(S): Nishimura, Haruki; Takamatsu, Hideji
CORPORATE SOURCE: Dainippon Pharm. Co., Ltd., Osaka, Japan
SOURCE: Yakugaku Zasshi (1964), 84(9), 811-17
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB Na2S2O3 and L-(+)-threo-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, followed by hydrolysis, gave (+)-1-phenyl-2-dimethylaminopropanethiol (I), which was then converted into the methiodide and treated with NaOH to form (+)-1,2-epithiopropylbenzene (II), b10 100°, which was polymerized to give a polymer, m. 255-6°. Treatment of D-(+)-erythro-1,2-epoxypropylbenzene with KSCN gave L-(-)-erythro-1,2-epithiopropylbenzene, b7 92-3°, [α]20D-21.4° (c 2.21, MeOH), which was found to be the antipode of II. II belongs to the D-(+)-erythro series and I, to the L-(+)-threo series. The (-)-amino thiol, similarly derived from L-(-)-erythro-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, was found to belong to the L-(-)-erythro series and that D-(+)-threo-1,2-epithiopropylbenzene (III) is derived from it. The steric configuration of II and III was also determined from their N.M.R. spectra. Hofmann degradation of the quaternary salt of 1-phenyl-2-dimethylaminoethanethiol also gave the same result. II and III underwent desulfurization by heating to give trans-β-methylstyrene.
IT 94960-76-6P, Phenethylamine, β,β'-dithiobis[α-methyl-, dihydrochloride, DL-threo-
RL: PREP (Preparation)
(preparation of)
RN 94960-76-6 CAPLUS
CN Phenethylamine, β,β'-dithiobis[α-methyl-, dihydrochloride (7CI) (CA INDEX NAME)



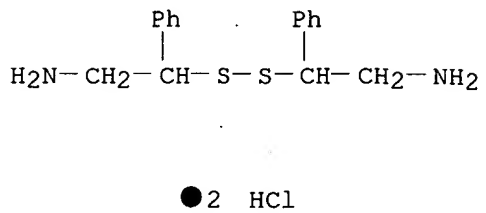
●2 HCl

L5 ANSWER 22 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:8902 CAPLUS
DOCUMENT NUMBER: 62:8902
ORIGINAL REFERENCE NO.: 62:1587d-h
TITLE: Phenylmercaptoalkylamines. I. 1-Phenyl-2(or 3)-amino-alkanethiol derivatives
AUTHOR(S): Nishimura, Haruki; Takamatsu, Hideji
CORPORATE SOURCE: Dainippon Pharm. Co., Ltd., Osaka, Japan
SOURCE: Yakugaku Zasshi (1964), 84(9), 797-805
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

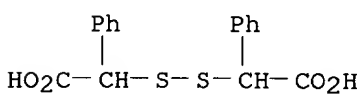
AB PhCH(OH)CH2R.HCl (1 part) is dissolved in 2 vols. CHCl3 and treated with a solution of SOCl2 (or PCl5) in CHCl3 under cooling to give the following PhCHClCH2R (I) (R, % yield, and m.p. of the hydrochloride given): NH2, 92, 164-5.5° (decomposition) (EtOH-Et2O); NHMe, 80, 175-6° (decomposition) (MeOH); NHEt, 63, 192° (decomposition) (iso-PrOH); NHPr, 94, 185-6° (iso-PrOH); iso-PrNH, 78, 185-6° (iso-PrOH); NMe2, 89, 206° (decomposition); NEt2, 100, --; NPr2, 48, 100.5-103° (AcOEt); iso-Pr2N, 55, 121-4° (AcOEt); pyrrolidino, 75, 181.5° (iso-PrOH); piperidino, 65, 178-9° (decomposition) (iso-PrOH); morpholino, 93, 188° (decomposition) (MeOH). Also prepared are PhCHCl(CH2)2NMe2, m. 176°, and PhCHCl(CH2)2Z (Z = piperidino), m. 151°. Equimolar mixture of I.HCl and Na2S2O3.5H2O in 1-2 vols. H2O is boiled 30-60 min. to give the following PhCH(SSO3H)CH2R (II) [R and m.p. (decomposition) given]: NH2, 213-14°; NHMe, 184°; NHEt, 192°; NHPr, 201°; iso-PrNH, 192°; NMe2, 207°; NEt2, 178°; NPr2, 204°; iso-Pr2N, 204°; pyrrolidino, 187°; piperidino, 206°; morpholino, 221°. I is treated with NaSH or II is treated with HCl to give the following PhCH(SH)CH2R (III) (R, b.p./mm., and m.p. hydrochloride given): NH2, 116-20°/7, 157-60°; NHMe, 98-104°/6 (m. 67-9°), 129-33°; NHEt, 100°/4, 173°; NHPr, 115-17°/5-6, 163°; iso-PrNH, 102-4°/4, 175-7°; NMe2, 109-12°/5, 184-5° (decomposition); NEt2, 109-12°/5.5, --; NPr2, 122-8°/5, --; iso-Pr2N, 115-18°/5, 148-50°; pyrrolidino, 116-19°/4, 177.5-8.5°; piperidino, 131-3°/4, 179-80° (decomposition); morpholino, --, 192-3° (decomposition). Oxidation of III gives the following (RCH2CHPhS)2 (R and m.p. of the dihydrochloride given): NH2, 210-13°; NHMe, 190-3° (decomposition); NHEt, 187-90°; NHPr, 202-4°; iso-PrNH, 186-90°; NMe2, 211° (decomposition); NEt2, 205-7°; NPr2, 209-10° (decomposition); iso-Pr2N, -- [free base m. 80-1° (MeOH)]; pyrrolidino, -- [free base m. 102-5° (ligroine)]; piperidino, -- [free base m. 78-9° (MeOH)]; morpholino, 205-8°. Also prepared are: PhCH(SH)(CH2)2NMe2 (b8 109-10°); PhCH(SH)(CH2)2Z (b5 148-50.5°); [Me2N(CH2)2CHPhS]2 (picrate m. 85-90°), and [Z(CH2)2CHPhS]2 (picrate m. 95-100°).

IT 3907-60-6P, Phenethylamine, β,β'-dithiobis-, dihydrochloride
RL: PREP (Preparation)
(preparation of)

RN 3907-60-6 CAPLUS
CN Benzeneethanamine, β,β'-dithiobis-, dihydrochloride (9CI) (CA INDEX NAME)



L5 ANSWER 23 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:16108 CAPLUS
DOCUMENT NUMBER: 56:16108
ORIGINAL REFERENCE NO.: 56:3016a-c
TITLE: Optical rotatory dispersion studies. XLII. Disulfides and diselenides
AUTHOR(S): Djerassi, Carl
CORPORATE SOURCE: Stanford Univ., Stanford, CA
SOURCE: Acta Chemica Scandinavica (1961), 15, 417-26
CODEN: ACHSE7; ISSN: 0904-213X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. CA 55, 10400f, 24515e. -Optical rotatory dispersion curves were determined for (XCH2CH(NH2)CO2H)2 and (XCHRCO2H)2, where X = S and Se and R = Me and Ph, (SeCHEtCO2H)2, (+)-1,2-dithiane-3,6-diearboxylic acid, (+)-1,2-diselenane-3,6-dicarboxylic acid, (-)-1,2-dithiane4-carboxylie acid, (+)-1,1'-binaphthalene 2,2'-disulfide, (-)-O,8-thioetic acid, la,Sa-epidithioaudrostane-3,17-dione, 1α,5α-epidithioandrostane-3α,17β-diol, and 3α,17β-dihydroxyandrostane-1α,5β-dithiol. The sterie relations of analogous disulfides and diselenides can be conveniently correlated by means of their dispersion curves, the same sign of the Cotton effects implying identical configuration.
IT 4695-07-2, Acetic acid, dithiobis[phenyl-
(optical rotatory dispersion of)
RN 4695-07-2 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)



L5 ANSWER 24 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:105470 CAPLUS
DOCUMENT NUMBER: 55:105470
ORIGINAL REFERENCE NO.: 55:19793a-c
TITLE: Nitro oxo alcohols and esters
INVENTOR(S): Klager, Karl
PATENT ASSIGNEE(S): Aerojet-General Corp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

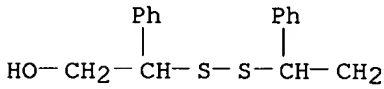
US 2978467		19610404	US 1957-635549	19570122

AB Nitro oxo alcohols, useful in the preparation of explosives, were prepared by condensing methyl vinyl ketone (I) with an active H-containing compound in the presence of NaOH or a mixture of H_2SO_4 and $HgSO_4$. Thus, 30 ml. of a 4% I solution was added during 10 min. to 3 g. nitroform (II) and 2 drops 20% aqueous NaOH in 10 ml. H_2O and after 3 days the solution was extracted with ether to yield 5,5,5-trinitro-2-oxopentanol, m. 77°, also prepared by heating 2-butyne-1,4-diol, H_2SO_4, and $HgSO_4$ in H_2O to 51 ± 1°, adding NaOAc to pH 5 after 1 hr. to produce I, adding the product to II and NaOH, and extracting with CH_2Cl_2. Similarly prepared from I and the indicated compound were 5,5-dinitro-2-oxohexanol, m. 27 ± 1°, from 2,2-dinitroethane; 5-nitro-5-methyl-2-oxohexanol from 2-nitropropane; 5,5-dinitro-2-oxoheptanol from 1,1-dinitropropane; 5,5-dinitro-2-oxooctanol from 1,1-dinitrobutane; Me 8-hydroxy-7-oxo-4,4-dinitrooctanoate from 4,4-dinitrobutyrate; 5-nitro-5-chloro-2-oxohexanol from 1-chloro-1-nitroethane; 5-nitro-5-cyclohexyl-2-oxohexanol from nitrocyclohexane.

IT 108843-15-8P, Phenethyl alcohol, β,β'-dithiodi-(?)
RL: PREP (Preparation)
(preparation of)

RN 108843-15-8 CAPLUS

CN Phenethyl alcohol, β,β'-dithiodi- (6CI) (CA INDEX NAME)



L5 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1958:35006 CAPLUS
DOCUMENT NUMBER:	52:35006
ORIGINAL REFERENCE NO.:	52:6257i,6258a-c
TITLE:	Synthesis of some derivatives of β-phenylcysteine
AUTHOR(S):	Sycheva, T. P.; Lebedeva, I. V.; Trupp, T. Kh.; Shchukina, M. N.
CORPORATE SOURCE:	S. Ordzhonikidze All-Union Chem. Pharm. Research Inst., Moscow
SOURCE:	Zhurnal Obshchei Khimii (1957), 27, 2287-92 CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE:	Journal
LANGUAGE:	Unavailable

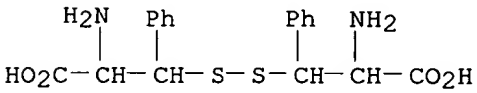
AB cf. Brown, et al., C.A. 49, 9093b. Passage of HCl into solution of phenylcysteine-HCl (I) in absolute EtOH gave the Et ester, m. 149-50°. This with Ph_3CCl in $CHCl_3$ gave the Et ester of N-tritylphenylcysteine, m. 154-6° (EtOH). I treated dropwise to neutral reaction with 18% NaOH gave after air blowing 1 hr. diphenylcystine, decompose 205-6°. Air blowing of solution of I Et ester gave diphenylcystine Et ester-2HCl, decompose 191°, which with BzCl gave Et ester of N,N'-dibenzoyldiphenylcystine, m. 147-9°. To 3 g. phenylserine Me ester-HCl and 30 ml. AcCl was added slowly 4.5 g. PCl_5 and after shaking 1 hr. the mixture was chilled overnight yielding 0.6 g. β-chlorophenylalanine Me ester-HCl, decompose 177° (EtOH-Et_2O). p-Nitrophenylserine Et ester-HCl with BzCl and Na_2CO_3 gave N-benzoyl-p-nitrophenylserine Et ester, m. 158-9°. Heating 5 g. N-benzoylphenylserine Et ester with 1.4 g. P_2S_5 to 110° 1.5 hrs. gave after 8 hrs. at 130° a mass which treated with EtOH, then with H_2O and extracted with Et_2O gave an oil which refluxed 7 hrs. with concentrated HCl

gave a low yield of C16H13O2NS.HCl, m. 165-6°, which treated with N NaOH, and rapidly acidified with AcOH gave 2,5-diphenyl-4-thiazolinecarboxylic acid, m. 140°. Phenylserine Me ester-HCl and Et3N in CHCl3 at 0°, followed by Ph3CCl gave after 1.5 days at room temperature N-tritylphenylserine Me ester, m. 136-8°. To 30 ml. liquid NH3, 2.56 g. I, and 1.23 g. diphenylcystine was added at -40° 0.9 g. Na, followed by 1.5 ml. MeI and after 2 hrs. the mixture yielded 2.5 g. S-methylphenylcysteine, m. 158-9°; HCl salt, m. 165-6°. Similar use of EtBr gave S-ethylphenylcysteine-HCl, m. 168-70°; the free amino acid, m. 153-4°. Similarly was prepared S-butylphenylcysteine, m. 157-9°; HCl salt, m. 155-7°. Attempts to prepare phenylcysteine from chlorocinnamic acid and CS(NH2)2 failed.

IT 102017-00-5, Alanine, 3,3'-dithiobis[3-phenyl- (and derivs.)

RN 102017-00-5 CAPLUS

CN Alanine, 3,3'-dithiobis[3-phenyl- (6CI) (CA INDEX NAME)



L5 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1957:9554 CAPLUS

DOCUMENT NUMBER: 51:9554

ORIGINAL REFERENCE NO.: 51:2036i,2037a-b

TITLE: 1-Allyloxy-2,4,6-tris(hydroxymethyl)benzene

INVENTOR(S): Burkhard, Charles A.

PATENT ASSIGNEE(S): General Electric Co.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

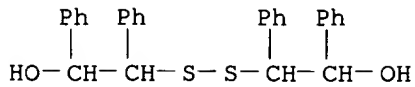
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2757208		19560731	US 1953-371401	19530730

AB 1-Allyloxy-2,4,6-trimethylolbenzene (I) was prepared by the hydrolysis of 1-allyloxy-2,4,6-tristrimethylsil-oxymethylbenzene (II). An aqueous solution of PhONa (188 g. PhOH, 90 g. NaOH, and 70 g. water) treated with 588 g. 37% HCHO, gave after 48 hrs. at less than 45°, and pouring into Me2CHOH 390 g. NaOC6H2(CH2OH)3-2,4,6 (III). III (200 g.), 500 ml. Me2CO (IV), 120 g. CH2:CHCH2Br (V), and 40 g. K2CO3 refluxed 7 hrs., filtered, and the excess IV and V were removed by evaporation are 148.4 g. impure I. Impure I (25 g.) in 150 ml. pyridine treated with 75 g. Me3SiCl, the excess pyridine and the hydrochloride were removed yielding II, b1 145°, nD20 1.4700. II 50, water 300, and MeOH 554 parts gave an exothermic reaction which after evaporation of the water, MeOH, and (Me3Si)2O gave I as a liquid, nD20 1.5603, and crystallized on cooling, m. 86-6.2°. I is useful as a polyol for polyester formation. Cf. C.A. 46, 3328b.

IT 35034-31-2P, Ethanol, 2,2'-dithiobis[1 2-diphenyl-
RL: PREP (Preparation)
(preparation of)

RN 35034-31-2 CAPLUS

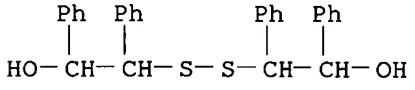
CN Benzeneethanol, β,β'-dithiobis[α-phenyl- (9CI) (CA INDEX NAME)



L5 ANSWER 27 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1957:9553 CAPLUS
DOCUMENT NUMBER: 51:9553
ORIGINAL REFERENCE NO.: 51:2036g-i
TITLE: Dithiodialkylene glycols
INVENTOR(S): McCarthy, John F., Jr.
PATENT ASSIGNEE(S): Thiokol Chemical Corp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2754333		19560710	US	

AB The title compds., (HOCHRCHR)2S2, where R is H, an alkyl, or an aryl group, are prepared by treating the corresponding alkylene oxide with H2S and S in an aqueous solution of alkali thiosulfate. Thus, ethylene oxide (I) and H2S are added simultaneously to 2.5 l. of 4M Na2S2O3 at a pH of 12.0-12.4 during 2 hrs.; the temperature rises to 44°. After standing overnight, the upper layer (169 g.) is separated, held at 20 mm. for 2 hrs. to remove excess H2S, and dried with Na2SO4 to obtain 140 g. dithiodiethanol (II). Mercaptan formation is favored by a lower pH. I and H2S may be added intermittently and alternately. Addition of 1 atom of S per mol. of H2S maintains a constant concentrate of thiosulfate. Further data on the conversions of I to II, propylene oxide to dithiodipropanol, and styrene oxide to dithiodiphenylethyl alc. are given in 11 other examples.
IT 35034-31-2P, Ethanol, 2,2'-dithiobis[1 2-diphenyl-
RL: PREP (Preparation)
(preparation of)
RN 35034-31-2 CAPLUS
CN Benzeneethanol, β,β'-dithiobis[α-phenyl- (9CI) (CA INDEX NAME)



L5 ANSWER 28 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1951:11202 CAPLUS
DOCUMENT NUMBER: 45:11202
ORIGINAL REFERENCE NO.: 45:1999b-i,2000a-i
TITLE: Syntheses in the penicillin field. IX. A synthesis of some penicillamine analogs and attempts to obtain new types of penicillins
AUTHOR(S): Cook, A. H.; Harris, G.; Pollock, J. R. A.; Swan, J. M.
CORPORATE SOURCE: Imperial Coll. Sci. Technol., London
SOURCE: Journal of the Chemical Society (1950) 1947-54
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 44, 4903g. EtSCSNHCH2CO2H (I) (2.5 g.), 2 g. Me2CO, and 6 cc. Ac2O, heated 15 min. on the steam bath, give only the unchanged I [PhNH2 in ether gives Nα-dithiocarbethoxyglycinanilide, m. 150-60° (decomposition)]. I (10 g.), 26 g. Me2CO, 20 g. Ac2O, and 5 g. AcONa, refluxed 3.75 hrs., give 2-ethylmercapto-4-isopropylidene-5(4H)-thiazolone, b0.2 110-15°; PhCH2NH2 in ether gives 1-benzyl-4-isopropylidene-2-thiohydantoin, m. 201°. PhCH.S.CS.NH.CHCOSH.Et3N (6.8 g.) and 35 cc. concentrated HCl, heated 16 hrs. at 90-100° (sealed tube), give 5-phenyl-4-thiazolecarboxylic acid-HCl, m. 225° (decomposition); the filtrate yields β-phenylcysteine-HCl (IA) (31% in 1 experiment); hydrolysis of the free carbothiolic acid gives the same products. I (3.6 g.), p-HOC6H4CHO, and 15 cc. Ac2O, heated 10 min. on the steam bath, give 19% 2-ethylmercapto-4-(p-acetoxybenzylidene)-5(4H)-thiazolone (II), pale orange, m. 108-10°; 1.8 g. I, 1.5 g. p-O2NC6H4CHO, and 5 cc. Ac2O, heated 3 min. at 100°, give 2 g. of the p-nitrobenzylidene analog of II, yellow, m. 161°. p-MeOC6H4CHO (20 g.) in 150 cc. boiling AcOH containing 20 g. 2-mercapto-5(4H)-thiazolone (III) and 10 drops morpholine, kept 2 hrs. at room temperature, gives 32 g. crude 4-(p-methoxybenzylidene) derivative (IV) of III, yellow, m. 212° (decomposition), which with Me2SO4-KOH yields the 2-methylmercapto compound, yellow, m. 124°. IV (5 g.) in 30 cc. MeOH containing 1 g. Na, kept 1 hr., poured into 150 cc. ice-cold 2 N HCl, kept 1 hr., and the gum in Me2CO at 0° cautiously treated with H2O, gives 2.8 g. Me 2-mercapto-5-(p-methoxyphenyl)-4-thiazolinecarboxylate (IVA), pale yellow, m. 108°. IV (37 g.) in 250 cc. hot MeOH containing 11 g. NaOH, kept 2.5 hrs. at room temperature, diluted with 1 l. H2O, and acidified with concentrated HCl, gives 28 g. 2-mercapto-5-(p-methoxyphenyl)-4-thiazolinecarboxylic acid, m. 149° (decomposition). IVA (2 g.) in 10 cc. 10% NaOH, treated with 10 cc. 20-volume H2O2, and kept 3 hrs., gives 1.2 g. 5-(p-methoxyphenyl)-2-thiazolidone-4-carboxylic acid, m. 138°. p-ClC6H4CHO (18 g.) and 16 g. III in 250 cc. hot AcOH containing 10 drops morpholine give 18 g. of the 4-(p-chlorobenzylidene) analog (V) of IV, orange, m. 250° (decomposition); 2-methylmercapto compound, golden, m. 145-6°; 2 g. V and 2 g. red P in 25 cc. AcOH and 10 cc. 40% HI, refluxed 4 hrs., give β-(p-chlorophenyl)cysteine (VA). 4-(p-Acetoxybenzylidene) analog (VI) of IV, yellow, m. 180° and then 196°; 2-methylmercapto compound, yellow, m. 114°; 5 g. VI in 20 cc. MeOH containing 2 g. Et3N, treated 12 hrs. with H2S and diluted with 250 cc. ether, gives 2.5 g. triethylammonium 2-mercapto-5-(p-acetoxyphenyl)-2-thiazoline-4-carbothiolate (VII), m. 127-8° (decomposition). 2-Mercapto-5-(p-hydroxyphenyl)-4-thiazolinecarboxamide (1 g.), refluxed 1 hr. with 10 cc. 2 N NaOH, gives 0.1 g. 2-mercapto-5-(p-hydroxyphenyl)-4-thiazolinecarboxylic acid (VIII), pale yellow, m. 196°; 2 g. VII in 5 cc. EtOH, treated with 2 cc. concentrated HCl, the resulting gum extracted with 20 cc. AcOEt and 10 cc. H2O, the aqueous layer extracted with 10 cc. AcOEt, the yellow oil from the AcOEt heated 3 hrs. with 10 cc. concentrated HCl, diluted with 30 cc. H2O, and extracted with AcOEt, gives 0.7 g. VIII, with 1 mol. AcOEt, m. 122° (decomposition); the AcOEt is lost on heating 18 hrs. at 100°/14 mm. VIII (20 g.), treated with CH2N2 in ether and the oil in 1 l. ether reduced with 30 g. Al-Hg, gives 6 g. Me 5-(p-methoxyphenyl)-4-thiazolidinecarboxylate (IX), m. 81°; Ac derivative, m. 94-5°; hydrolysis of 0.4 g. IX with 20 cc. 4 N HCl (13 hrs.) gives 0.4 g. of the HCl salt, m. 193-6° (decomposition), of the free acid, m. 210° (decomposition). IX (2.5 g.) in 10 cc. MeOH, added to 5 g. HgCl2 in 300 cc. MeOH, refluxed 1 hr., concentrated, decomposed with H2S, and the yellow oil treated with (CO2H)2, gives 0.7 g. bis[2-amino-2-carbomethoxy-1-(p-methoxyphenyl)ethyl] disulfide bis(H oxalate), m. 148°. IX (by the method given below) gives β-(p-methoxyphenyl) cysteine-HCl, m. 166°, indigo-blue color

with FeCl3, red-purple color with ninhydrin. III and 11 g. p-AcOC6H4CHO with 4 drops of piperidine in AcOH give 0.8 g. p-ClC6H4CH2CH(NH2)CO2H, m. 253° (decomposition). V (30 g.) in 100 cc. hot MeOH containing 9 g. KOH, kept 0.5 hr., diluted to 500 cc., acidified, kept 12 hrs. at 0°, and the oil in AcOEt extracted with NaHCO3 and acidified, gives 2-mercapto-5-(p-chlorophenyl)-5-thiazolinecarboxylic acid, m. 176°; methylation and reduction with Na-Hg give Me 5-(p-chlorophenyl)-4-thiazolidinecarboxylate (X), m. 114-15°. X (1 g.) in 10 cc. EtOH, heated to boiling, diluted with 100 cc. H2O at 60°, and added to 2.5 g. HgCl2 in 100 cc. hot H2O, gives the HCl salt of VA, m. 177° (decomposition), purple color with FeCl3, red-purple color with ninhydrin. The HCl salt of VA (2.3 g.) and 2.6 g. AmCONHCH(CHO)CO2Et, heated 10 min. at 100° with a few drops MeOH and the resin triturated with ether containing a little HCl, give the HCl salt (XI), m. 179° (decomposition), of 5-phenyl-2-[(hexanoylamino)carbethoxymethyl]-4-thiazolidinecarboxylic acid (XII), m. 135°. VA (1 g.), 1.5 g. PhCH2CONHCH(CHO)-HO2CCH-NH CO2Et PhCH.S.CH-CHNHCOAm (XII) CO2Et, and 1 cc. MeOH, heated 12 min. at 100°, give the HCl salt, amorphous, m. 100° (decomposition), of the (phenylacetamido) analog of XII, m. about 130° (decomposition) (mixture of stereoisomers). XI (3.9 g.) in 52.5 cc. 0.509 N NaOH, kept 23 hrs., treated with 1.58 g. AcOH and 12 cc. 30% Pb(OAc)2 at 0°, and the Pb salt decomposed (20 min.) in EtOH with H2S, give 2.35 g. 5-phenyl-2-[(hexanoylamino)-carboxymethyl]-4-thiazolidinecarboxylic acid (XIII), m. 108° (decomposition); XIII could not be converted to an azlactone with Ac2O alone or with C5H5N or Et3N (the product had no bacteriostatic activity). Attempted condensation of VA (or the p-Cl or p-MeO derivs.) with 2-benzyl-4-(ethoxymethylene)oxazolone did not yield products with antibiotic activity. H2NCH2CO2Et.HCl (0.347 g.) in 5 cc. Me2CO and 2.27 cc. 1.1 N KOH, treated with 0.472 g. 2-mercapto-4-ethoxymethylene-5(4H)-thiazolone (XIV) in 20 cc. warm Me2CO, kept 2.5 hrs. at room temperature, 15 cc. Me2CO added, and the mixture kept overnight, gives 0.52 g. 2-mercapto-4-{[(carbethoxymethyl)amino]methyl}-5(4H)-thiazolone, yellow, m. 210° (decomposition), absorption maximum at 2450 and 3370 A. (E1%1 cm. 400 and 570). H2NCH2CO2H (0.187 g.) in 5 cc. Me2CO and 30 cc. H2O containing 2.27 cc. 1.1 N KOH, treated with 0.47 g. XIV in 20 cc. warm Me2CO, shaken 2 hrs., kept 26 hrs., and treated with 2.65 cc. 0.943 N HCl, gives 0.45 g. 2-mercapto-4-{[(carboxymethyl)amino]methylene}-5(4H)-thiazolone, m. 222° (decomposition), absorption maximum at 2470 and 3390 A. (E1%1 cm. 450 and 590). MeCH(NH2)CO2Me (0.347 g.) gives 0.45 g. 2-mercapto-4-[(1-carbomethoxypropylamino)methylene]-5(4H)-thiazolone, yellow, m. 210-11° (decomposition), absorption maximum at 2450, 2500, and 3640 A. (E1%1 cm. 470, 450, and 660). S-Benzylpenicillamine (0.597 g.) gives 0.95 g. 2-mercapto-4-[(1-carboxy-2-benzylmercapto-2,2-dimethylpropylamino)methyl]-5(4H)-thiazolone, yellow, m. 220° (decomposition), absorption maximum at 2450 and 3440 A. (E1%1 cm. 390 and 490). XIV (1.89 g.) and 1.24 g. PhCH2SH in 1 cc. Et3N, heated 5 min. at 100° and the product (0.7 g.) recrystd. from AcOH and EtOH, give 2 isomers of 2-mercapto-4-benzylmercaptomethylene-5(4H)-thiazolone, yellow, m. 185°, absorption maximum at 2600, 2970, and 3650 A. (E1%1 cm. 215, 195, and 500), and m. 143°; crystallization from AcOH caused partial conversion into the higher-melting product. The Na salt of XIV in H2O or XIV in EtOH with penicillamine [Na salt or Me ester (XV)] gives only amorphous, easily oxidized salts. XV.HCl and XIV do not react on refluxing in CHCl3, C6H6, or AcOEt or on heating at 100° in PhOMe; decomposition occurs in boiling PhOMe; condensation does not occur in 6 N HCl or MeOH-HCl. Other derivs. of penicillamine do not react.

IT 900498-22-8P, Oxalic acid, compound with 3,3'-dithiobis(3-(p-methoxyphenyl)alanine]
RL: PREP (Preparation)
(preparation of)

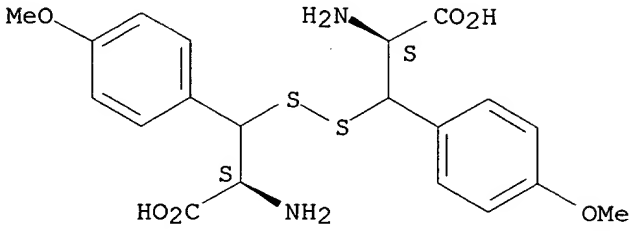
RN 900498-22-8 CAPLUS

CN Oxalic acid, compd. with 3,3'-dithiobis(3-(p-methoxyphenyl)alanine] (5CI) (CA INDEX NAME)

CM 1

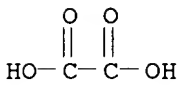
CRN 900498-21-7
CMF C20 H24 N2 O6 S2

Absolute stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

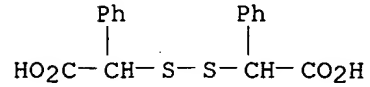


L5 ANSWER 29 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1936:45170 CAPLUS
DOCUMENT NUMBER: 30:45170
ORIGINAL REFERENCE NO.: 30:5983i,5984a-c
TITLE: Alkaline fission of disulfides. II. The hydrolytic fission of the disulfide linkage
AUTHOR(S): Schoberl, Alfons; Eck, Hubert
SOURCE: Ann. (1936), 522, 97-115
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

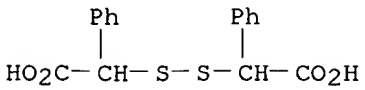
AB cf. C. A. 29, 143.1. Alkaline hydrolysis of [RCH(CO2H)S]2 gives RCH(CO2H)SH (I) and RCH(CO2H)SOH (II); II yields H2S and ROCCO2H (III); if in III R is CO2H or CH2CO2H, the compound loses CO2 to give CHOCO2H or AcCO2H. II (2 mols.) may yield I and RCH(CO2H)SO2H. III is detected by the use of Pb(OAc)4 and addition of p-H2NNHC6H4CO2H (IV); acidification gives p-HO2CC6H4NHN:CRCO2H. Under these conditions diphenyldithiodiglycolic acid yields 25.6% of phenylglyoxylic acid p-carboxyphenylhydrazone, yellow, m. 217-19°. [SCH(CO2H)2]2 and (SCH2CO2H)2 give 49.3 and 50% of glyoxylic acid p-carboxyphenylhydrazone, decomposing above 265° (also prepared from Cl2CHCO2H and IV in concentrated KOH), while (SCHMeCO2H)2 and α,α'-disulfidodisuccinic acid (V) give 67.5 and 32% of pyruvic acid p-carboxyphenylhydrazone (VI), yellow, decomposing 236° (di-Me ester, m. 166°). A neutral solution of the Na salt of V is hydrolyzed on boiling; with IV there results 1-(4'-carboxyphenyl)-5-pyrazolone-3-carboxylic acid (VII) (Me ester, m. 242° (decomposition)) and some VI. IV and HO2CCOCH2CO2H in neutral solution give VII and VI, while in acid solution only VII results. The Me ester of the 3-carboxyphenyl ester m. 198° (decomposition). Hydrolysis of [PhCH2CH(CO2H)S]2 (preparation given) gives α-thiocinnamic acid, m. 128°.

IT 4695-07-2, α-Toluic acid, α,α'-dithiobis-

(hydrolysis of)
RN 4695-07-2 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)



L5 ANSWER 30 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1935:1121 CAPLUS
DOCUMENT NUMBER: 29:1121
ORIGINAL REFERENCE NO.: 29:143a-f
TITLE: The alkaline cleavage of disulfides. I. Behavior of diphenyldithiodiglycolic acid
AUTHOR(S): Schoberl, Alfons; Berninger, Emil; Harren, Franz
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1934), 67B, 1545-50
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A. 28, 105.6. This work was undertaken to obtain light on the mechanism of the splitting off of H2S from cystine with alkalies. Evidence had already been presented that the primary process in the cleavage of aliphatic disulfides of a definite type with alkalies consists in a hydrolytic rupture of the disulfide union with formation of a sulfhydryl compound and a sulfenic acid: HO2C.R.-S.S.R.CO2H + HOH → HO2C.R.SH + HO.S.R.CO2H. Dithiodiglycolic and dithiodilactylic acids had been split in this way and the detection and isolation of the resulting sulfhydryl compds. in general offered no difficulties. The sulfenic acids, however, may give rise to complications because of their instability and reactiveness. Possibly they are stabilized by the splitting off of H2S; the HO2C-CH2SOH formed from dithiodiglycolic acid would then give HO2CCHO which in the alkaline medium would at once undergo a Cannizzaro disproportionation, and (CO2H)2 was actually obtained. No definite proof of such a mechanism was available, however, and it was thought diphenyldithiodiglycolic acid (I) might be well adapted to furnish such proof. I is best prepared from PhCHBrCO2H and Na2S2, both the dl- and meso-forms being obtained. If any rise in temperature is avoided, the reaction proceeds smoothly, whereas in the heat only mandelic acid is formed. As was to be expected, I is exceedingly unstable toward alkalies, which hydrolyze it to PhCH(SH)CO2H (II) (obtained in about 50% yield) and PhCH(SOH)-CO2H (III), and the III loses H2S to form PhCOCHO (isolated in 45.5% yield). The mechanism of the alkaline cleavage of I explains also its degradation by O in alkaline solution which is characterized by a vigorous and plentiful absorption of O and the formation of PhCOCO2H. The latter, however, is not an oxidation product; the O is consumed chiefly in oxidizing the Na2S to Na2S2O3. Much BzOH is formed along with the PhCOCO2H. From 60 g. PhCHBrCO2H with Na2S2 are obtained 29 g. of I, needles and leaflets, m. 218°, and 1.15 g. of an isomer m. around 141° which seps. from water in leaflets with 1 H2O. Both forms are also obtained by oxidation of II with I.
IT 4695-07-2P, α-Toluic acid, α,α'-dithiobis-
RL: PREP (Preparation)
(preparation of)
RN 4695-07-2 CAPLUS
CN Benzeneacetic acid, α,α'-dithiobis- (9CI) (CA INDEX NAME)



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EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
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L2	8425	WOLFF.in. or MONAHAN.in. or BUDKER.in. or SLATTUM.in. or ROZEMA.in.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	ADJ	ON	2007/03/15 14:29
L3	236	l2 and disulfide	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	ADJ	ON	2007/03/15 14:29
L4	69	l3 and glutathione	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	ADJ	ON	2007/03/15 14:30
L5	123	l3 and crosslinking	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	ADJ	ON	2007/03/15 14:31
L6	95	l5 and thiol	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	ADJ	ON	2007/03/15 14:31
L7	0	l6 and electronwithdrawing	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	ADJ	ON	2007/03/15 14:32
L8	19	l6 and electron withdrawing	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	ADJ	ON	2007/03/15 14:32